A STUDY of INELASTIC ELECTRON-PHONON INTERACTION ON TUNNELING MAGNETORESISTANCE IN POLYACETYLENE

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ABSTRACT

In this research, we study the effect of inelastic electron-phonon interactions on magneto-transport properties of a sandwiched Polyacetylene molecule between two ferromagnetic electrodes by using a modified Green's function method. The molecule is described with the well-known Su–Schrieffer–Heeger Hamiltonian in the tight binding form. The self-energy of electrodes is written in the wide-band approximation and spin-flip is neglected during conduction process. Our calculation results show that with increasing of voltage current increases and tunneling magnetoresistance (TMR) is decreased. The changes in TMR due to the inelastic interaction is limited in a small bias voltage interval and can be neglected in the other bias voltages. These results confirm the neglecting of inelastic interactions in previous theoretical works.

Keywords: tunneling magnetoresistance; Green's function; Polyacetylene; inelastic electron-phonon interaction.

INTRODUCTION

Due to its application in electronic devices, transport trough molecule has been studied in detail, both theoretically and experimentally. Theoretical and experimental works confirm that conducting polymers can act as spin-polarized materials [1-4]. We have use the SSH Hamiltonian which a well-known Hamiltonian for the calculation of electronic and transport properties of organic semiconductors [1,4,5]. In the presence of magnetic field, the magnetic of electrodes are oriented in the same direction and the scattering for spin up decreases while increases for spin down. By considering a parallel circuit in conduction with different spins, the presence of magnetic field can make a short circuit and as a result conduction of system decreases. In this work, we study spin dependent transport in a Polyacetylene molecule in the presence of inelastic electron-phonon interactions. We sandwiched a Polyacetylene molecule between two cobalt electrodes as we have schematically shown in *Figure 1*. Because of the weakness in spin-orbit coupling and hyperfine

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interactions in the organic materials, spin relaxation length is long and spin-flip process during conduction can be neglected [2, 6]. The presence of phonon in the finite temperature changes the transmission mechanisms which is neglected in many previous works. Here, we study the effect of inelastic interactions in the central region and neglect the interaction in leads. Walczak developed a Green's function approach to study the electron transport through DNA molecule in the presence of electron-phonon interactions [7, 8]. We had used the same formalism to study the inelastic electron phonon interaction in organic molecules. In this work we will use the same approach for the Polyacetylene molecule.

MODEL AND METHODS

The electronic part of Hamiltonian can be written as,

$$H = \begin{pmatrix} H_L & H_{L,C} & 0 \\ H_{L,C}^{+} & H_C & H_{R,C}^{+} \\ 0 & H_{R,C} & H_R \end{pmatrix} \tag{1}$$

where $H_{L/R}$ denotes Hamiltonian of left/right electrode and H_C represents molecular Hamiltonian. Other matrix elements show the coupling between electrodes and scattering region. Both electrodes are described in the wide-band approximation [7,8].

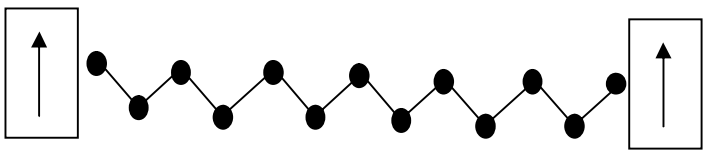

Fig. 1 –Schematic representation of Polyacetylene molecule sandwiched between two electrodes

The Polyacetylene molecule which is considered as a quasi-one-dimensional chain with N pair of carbon atoms can be described by means of modified SSH Hamiltonian as follows [1,9],

$$H_M = -\sum_{n=1}^{2N}\sum_{\sigma}[(t_0 + \alpha(u_n - u_{n+1}))(d_{n,\sigma}^{+} d_{n+1,\sigma} + d_{n+1,\sigma}^{+} d_{n,\sigma})] \tag{2}$$

where t_0 is the hopping integral in a undimerized molecule and and u_i is the displacement of the *i*th Carbon atom. The index *i* runs over the orbitals of Carbon chain of molecule. The operator C_i (C_i^{+}) creates/annihilates a π electron with spin σ at the *i*-th site of Polyacetylene molecule.

The electron-phonon coupling constant is denoted by α. The electronic states in the Polyacetylene chain accompanied with m phonons can be written as [7, 8],

$$|n\sigma, m\rangle = d^{+}_{n\sigma} \frac{(a^{+})^{m}}{\sqrt{m!}} |0\rangle \tag{3}$$

a_i and a_i^{+} are phonon creation and annihilation operators, respectively and $|0\rangle$ shows the vacuum state. For the sake of simplicity, we consider only one phonon mode with energy *w*. In this new basis the Hamiltonian of the Polyacetylene can be written as,

$$H_M = \sum_{n,j,\sigma} [\varepsilon_{n\sigma} - \lambda(a_j + a_j^{+})] d^{+}_{n,\sigma} d_{n,\sigma} - [(t_0 + \alpha(u_n - u_{n+1}))(d^{+}_{n,\sigma} d_{n+1,\sigma} + d^{+}_{n+1,\sigma} d_{n,\sigma})] \tag{4}$$

where λ is the energy of electron-phonon interaction, in this work we assume that $|\lambda|=|\alpha|$. In the absence of inelastic electron-phonon interactions during conduction process, electron states will be changed from $|1, m\rangle$ to $|4N, m\rangle$. But in the presence of inelastic interactions, electrons can absorb/emit phonon and conduct between two levels with different number of phonons, for such a process we can write transmission coefficient as [7],

$$T^{\sigma,\sigma'}_{m,m'}(\varepsilon) = \Gamma^{\sigma}_{L} \Gamma^{\sigma'}_{R} \, | G^{\sigma,\sigma'}_{m+1,m'+1} |^2 \tag{5}$$

where $\Gamma^{\sigma}_{L/R} = 2\pi \, | \gamma_{L/R} |^2 \, \rho^{\sigma}_{L/R}$ (γ_α is the coupling strength between molecule and electrodes, ρ^{σ} is the density of state in the electrodes for spin σ) and the Green's function is defined as follows [1, 7, 8],

$$G^{\sigma,\sigma'}(\varepsilon) = [E - H_M - \Sigma^{\sigma}_{L} - \Sigma^{\sigma'}_{R}]^{-1} \tag{6}$$

All the off-diagonal terms in the Hamiltonian which are described the interaction between molecule and leads are compressed in the self-energy terms. The real part of self-energy is simply a shift in energy axis but the imaginary part describes the coupling of molecule with electrodes. In the wide-band approximation the real part of self-energy is neglected and the imaginary part is assumed an energy independent term which is written as $\Sigma^{\sigma}_{L/R} = \frac{\mathrm{i}}{2} \Gamma^{\sigma}_{L/R}$. The total transmission can be defined as a sum over all incoming/outgoing channels with different number of phonon in the initial and final sites. Each transmission mechanism is weighted by an appropriate factor P_m, which is the Boltzmann distribution function [7, 8].

$$T_{tot}(\varepsilon) = \sum_{m,m',\sigma} \mathrm{P}_m T^{\sigma,\sigma'}_{m,m'}(\varepsilon)$$

(7)

From the above equation the elastic part of transmission occurs when m and m' are equal and can be written as [7, 8],

$$T_{ele}(\varepsilon) = \sum_{m,\sigma} \mathrm{P}_m T_{m,m}^{\sigma,\sigma'}(\varepsilon) \tag{8}$$

The total current through junction is derived as follows,

$$I_{tot} = \frac{1}{2\pi} \int_{+\infty}^{-\infty} d\varepsilon \sum_{m,m',\sigma} T_{m,m'}^{\sigma,\sigma'} [\mathrm{P}_m f_L^m (1 - f_R^{m'}) - \mathrm{P}_{m'} f_R^{m'} (1 - f_L^m)] \tag{9}$$

The elastic part of current can be obtained from the above equation by the assumption of m=m' [7,8],

$$I_{ele} = \frac{1}{2\pi} \int_{+\infty}^{-\infty} d\varepsilon \sum_{m,\sigma} T_{m,m}^{\sigma,\sigma'} \mathrm{P}_m [f_L^m - f_R^m] \tag{10}$$

where $f_{L/R}^m$ is the Fermi function of the left/right electrode in applied voltage *V,* with chemical potential $\mu_{L/R}=\varepsilon_f \pm (eV/2)$ and Fermi energy ε_f.

We calculate transmission coefficient in the presence $T^{\sigma,\sigma}$ and absence $T^{\sigma,-\sigma}$ of magnetic field. Total current and elastic part of current can be calculated from Equations (9) and (10). Finally, tunneling magnetoresistance can be defined as the change in the current due to the external magnetic field by using the following equation [11],

$$TMR(V) = \frac{I_p(V) - I_{AP}(V)}{I_P(V)} \tag{11}$$

where I_p (I_{Ap}) is the current in the presence/absence of magnetic field. Calculations are performed for the total current and elastic part of current and then we have compared the TMR in these two situations.

RESULTS AND DISCUSSION

Numerical calculations are carried out for a molecule with 15 carbon pairs (30 sites) and the parameters for a Polyacetylene chain are chosen as (given in eV): t_0=2.5, α= 4.1 1/Å and u=0.04 A°. These parameters well describe a Polyacetylene chain. We have used the following set of parameters for describing Cobalt electrodes (given in 1/eV), $\rho^{\uparrow}$=0.1367, $\rho^{\downarrow}$= 0.5772, and we set $\gamma_L=\gamma_R$=0.2 eV, ε_f =-1 eV and w=0.1 eV. By increasing the number of phonons in each site the Boltzmann factor tends to zero as a result considering a finite number of phonons in each site is a reasonable assumption. Here**,** Maximum number of allowed phonon quanta is chosen to be five and all of the calculations are done at room temperature. We also assume that the external magnetic field does not change the electronic structure of molecule and the

changes are restricted in the electrodes region. In the presence of magnetic field, density of states in electrodes and transmission coefficient through the molecule are different for each spin. The presence of inelastic interactions emission and absorption of phonons activate new transmission mechanism. These new mechanisms are spin independent phenomena and change the magneto transport trough the molecule.

Figure 2 shows the current-voltage characteristic of Polyacetylene molecule in the presence of magnetic field. According to current–voltage characteristic of Polyacetylene it can be suggested as a switch in electronic circuit.

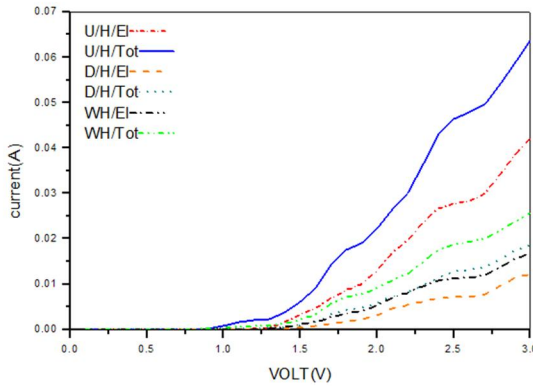

Fig. 2 –The total (T) and elastic (E) part of current as a function of bias voltage for electrons with spin up (U) and spin down (D) in the presence of magnetic field

Figure 3(a) presents TMR versus bias voltage in the presence and absence of inelastic electron-phonon interactions. The difference between these them is plotted in Fig. 3(b).

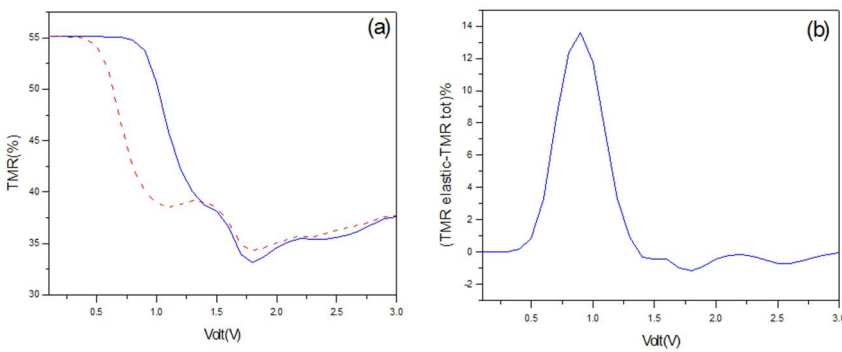

Fig. 3 – (a) Elastic part (solid line) and total (dashed line) of TMR (b) difference between these situations

As we expected, due to spin independent nature inelastic electron phonon interaction TMR decreases. In the low voltage regime the tunneling probability is near zero, current is small and TMR is constant. By increasing voltage energy-window opens and resonant tunneling occurs and as a result, current increase while TMR decreases. The polaron formation due to the electron phonon interaction shifts the current peak and reduces the conductance gap [12]. As a result the damping of TMR is occurred in a lower voltage. At higher voltages, TMR does not change with the increase of voltage. By increasing the applied voltage the energy of electrons is increases and the changes made by inelastic interactions are disappeared. A comparison between these results and our previous results for Polythiophene [13] confirms the neglecting of inelastic electron phonon interaction in the transport calculation of organic molecule, even in room temperature.

CONCLUSIONS

In summary, we have investigated the effect of inelastic electron-phonon interactions on the magneto transport in a Polyacetylene molecule. Our calculations indicate that the change of TMR due to inelastic interaction is limited in a small bias voltage interval and can be neglected in other bias voltages. These results confirm the neglecting of the inelastic interactions in previous theoretical works.

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